Message

From: Gaines, Linda [Gaines.Linda@epa.gov]
Sent: 10/19/2017 6:54:39 PM
To: Strynar, Mark [Strynar.Mark@epa.gov]; Libelo, Laurence [Libelo.Laurence@epa.gov]; Lau, Chris [Lau.Christopher@epa.gov]; Patlewicz, Grace [Patlewicz.Grace@epa.gov]; Surapureddi, Sailesh [surapureddi.sailesh@epa.gov]; Donohue, Joyce [Donohue.Joyce@epa.gov]; Volz, Stephanie [Volz.Stephanie@epa.gov]
Subject: RE: PFAS structural sub-workgroup
Attachments: PFAS structures.pptx

It is freeware UNLESS you are government? That is new.

The mol file that I can download from molview is easier for you to use than SMILES or InChIKey? I ask because I have all the SMILES and InChIkey recorded on a spreadsheet. [I think there are about four where I have the SMILES but can't get an InChIKey.

This is what I have put together so far. Not done yet, but you can see what I have put together. If we want to add other models to this, that is fine with me. It occurred to me I only have the linear versions on here. I can't draw every branched version because that is simply way too many structures. I could draw a couple though. The n-1 methyl version seems to be common enough that several PFAS have a CASRN for that version. I asked a couple of chemists at the conference I have been at this week, if they could tell me the most common branched. No real definitive answer on that.

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From: Strynar, Mark
Sent: Thursday, October 19, 2017 2:09 PM
To: Gaines, Linda <Gaines.Linda@epa.gov>; Libelo, Laurence <Libelo.Laurence@epa.gov>; Lau, Chris <Lau.Christopher@epa.gov>; Patlewicz, Grace <Patlewicz.Grace@epa.gov>; Surapureddi, Sailesh <surapureddi.sailesh@epa.gov>; Donohue, Joyce <Donohue.Joyce@epa.gov>; Volz, Stephanie <Volz.Stephanie@epa.gov>
Subject: RE: PFAS structural sub-workgroup

We use ACD Labs ChemSketch for all of our drawings of chemical structures. We have a site license through NCCT. Send me a mol file and I can send back some additional van der waals spheres. It is freeware unless you are government.

Mark

From: Gaines, Linda
Sent: Tuesday, October 17, 2017 11:37 AM
To: Strynar, Mark <Strynar.Mark@epa.gov>; Libelo, Laurence <Libelo.Laurence@epa.gov>; Lau, Chris <Lau.Christopher@epa.gov>; Patlewicz, Grace <Patlewicz.Grace@epa.gov>; Surapureddi, Sailesh <surapureddi.sailesh@epa.gov>; Donohue, Joyce <Donohue.Joyce@epa.gov>; Volz, Stephanie <Volz.Stephanie@epa.gov>
Subject: RE: PFAS structural sub-workgroup

Quick question for all: At Chris's request, I have been compiling the 3-D structures. I have been using molview.org using the van der Waals spheres for this. Does anyone know of any software we have access to or another free website I can

use that would produce better models? These models might be perfectly good, but I just thought I would check to see if anyone has preferences or opinions on this.

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From: Gaines, Linda
Sent: Thursday, October 12, 2017 9:22 AM
To: Strynar, Mark <strynar.mark@epa.gov>; Libelo, Laurence <Libelo.Laurence@epa.gov>; Lau, Chris <Lau.Christopher@epa.gov>; Patlewicz, Grace <Patlewicz.Grace@epa.gov>; Surapureddi, Sailesh <Surapureddi.Sailesh@epa.gov>; Donohue, Joyce <Donohue.Joyce@epa.gov>; Volz, Stephanie <Volz.Stephanie@epa.gov>
Subject: RE: PFAS structural sub-workgroup

Mark,

Very helpful. Thank you. I did not see anything about those two additional Nafion chemicals in your published article from 2015 or the letter that was sent to NCDEQ about the analytical results. Those were the two sources I was using for most of the Chemours stuff. Do you think these two other ones may be found in the environment?

Also, to be clear, this exercise of mine drawing the structures was more about me keeping these things straight and potentially helping some of the regional people trying to work on sites with these different things. I thought it could help this workgroup though.

Chris asked if I could get 3D drawings of the molecules to help model docking. I think I found a way to do that, so I will be exploring that next.

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From: Strynar, Mark
Sent: Thursday, October 12, 2017 8:30 AM
To: Gaines, Linda <Gaines.Linda@epa.gov>; Libelo, Laurence <Libelo.Laurence@epa.gov>; Lau, Chris <Lau.Christopher@epa.gov>; Patlewicz, Grace <Patlewicz.Grace@epa.gov>; Surapureddi, Sailesh <surapureddi.sailesh@epa.gov>; Donohue, Joyce <Donohue.Joyce@epa.gov>; Volz, Stephanie <Volz.Stephanie@epa.gov>
Subject: RE: PFAS structural sub-workgroup

Linda,

I have looked at all structures. I cannot comment on the AFFF compounds as I am not really informed about those. However, all structures I looked at appeared correct. I had a few minor changes in red for the analytes associated with GenX or the Nafion byproducts.

Also see the attached PPT slide. We believe these 2 chemicals (called the Nafion monomer and Nafion Monomer precursor) are both contributing to Nafion BP1 and BP2 in the water here in NC. Not sure if both should be included here.

Mark

From: Gaines, Linda
Sent: Wednesday, October 11, 2017 5:37 PM
To: Libelo, Laurence <Libelo.Laurence@epa.gov>; Lau, Chris <Lau.Christopher@epa.gov>; Patlewicz, Grace <Patlewicz.Grace@epa.gov>; Surapureddi, Sailesh <surapureddi.sailesh@epa.gov>; Donohue, Joyce <Donohue.Joyce@epa.gov>; Volz, Stephanie <Volz.Stephanie@epa.gov>; Strynar, Mark <Strynar.Mark@epa.gov>
Subject: PFAS structural sub-workgroup

Hi all,

First of all, most of you have already said you had no comments on the draft objectives list. Thank you. If you have not already looked at them, or you just want another look, please do so by COB 10/13. I will then send them to Lynn and Kathleen. They will then be shared with the larger options workgroup.

Ex. 6 Personal Privacy (PP)

Second, I mentioned this to some of you that I have been working on getting the structures drawn for many PFAS. Currently what I have drawn is the more standard PFAS (i.e. carboxylic acids, sulfonates, etc.), some of the GenX/Nafion products and byproducts, and some of the more complex PFAS that are associated with AFFF and who knows what else. My understanding is greatly increased by seeing structures. I am sharing in case it may help you. However, I would really appreciate it if you could also take a look and let me know if there are any inaccuracies. [Mark, please especially look at the GenX stuff.] Laurence, are there any structures you think I should add? I recall a poster of yours with another class of them that I do think I captured here.

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